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Comparisons of laboratory wavelength measurements with theoretical calculations for neon-like through lithium-like argon, sulfur and silicon

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Abstract

Atomic structure codes have a difficult time accurately calculating the wavelengths of many-electron ions without the benefit of laboratory measurements. This is especially true for wavelengths of lines in the extreme ultraviolet and soft X-ray regions. We are using the low-energy capability of the Livermore electron beam ion traps to compile a comprehensive catalog of astrophysically relevant emission lines in support of satellite X-ray observations. Our database includes wavelength measurements, relative intensities and line assignments, and is compared to a full set of calculations using the Hebrew University – Lawrence Livermore Atomic Code (HULLAC). Mean deviation of HULLAC calculations from our measured wavelength values is is highest for L-shell transitions of neon-like ions and lowest for lithium-like ions, ranging from a mean deviation of over 500 m Å for Si V to 12 mÅ in Ar XVI.

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1. Introduction

Satellite observations in the extreme ultraviolet and soft X-ray spectral regions provide unique and valuable diagnostic opportunities for astronomers and astrophysicists, containing a wealth of emission lines that can be used for determining plasma

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properties and elemental abundances over a wide temperature range. Observations in the soft X-ray region by the *Chandra X-ray Observatory* and *XMM-Newton* are now providing high-resolution spectra. There are many more lines in these spectra than can be currently identified, as is illustrated by *Chandra* spectra of Capella [1] and Procyon [2]. A wealth of mostly weak lines, presumably from L-shell ions of magnesium, silicon, sulfur, argon and calcium, remains largely unassigned as calculations cannot provide wavelengths of sufficient accuracy for unequivocal identification. The accuracy of the calculated wavelengths is limited because the structure of the intermediate ionization stages of ions of astrophysical interest are significantly affected by electron–electron interactions, and these ionization stages must be calculated in intermediate coupling. In the following we compare laboratory measurements of the L-shell transitions of argon, sulfur and silicon to theoretical wavelengths computed with the HULLAC set of atomic computer codes and assess their accuracy.

2. Experiment

Spectroscopic measurements were made on the University of California, Lawrence Livermore National Laboratory electron beam ion traps, EBIT-I and EBIT-II, which can be operated at the very low voltages (100–1000 eV) necessary to produce the charge states of interest. Different charge states can be produced simply by changing the voltage of the electron beam. As the voltage increases, higher charge states appear when their ionization potentials are exceeded, and lower charge states decline and disappear as they become ionized and "burn out". Our electron beam ion traps operate at a density of $\sim 10^{11}$ cm^{-3}, i.e. in the collisionless regime, similar to that of many astronomical plasmas, such as stellar coronae and supernova remnants.

Spectra shown were taken with either of two grazing-incidence spectrometers combined with a CCD camera having a one inch square array of 1024×1024 pixels and either a 1200 ℓ/mm or a 2400 ℓ/mm grating [3,4]. The spectra were calibrated using the well known K-shell emission lines of nitrogen, carbon and oxygen. These lines were observed in the second through seventh orders (49–173 Å) with the 1200 ℓ/mm spectrometer and in first order (19–40 Å) with the 2400 ℓ/mm spectrometer. Fig. 1 shows part of a spectrum of silicon taken at a beam energy of 300 eV. The dominant lines in the spectrum are from neon-like Si V, fluorine-like Si VI and oxygen-like Si VII. Synthetic spectra from from HULLAC calculations are overlaid to demonstrate the level of accuracy of calculations for these ions in this wavelength region. From Fig. 1 it is clear that line assignments are essentially impossible unless one experimen-

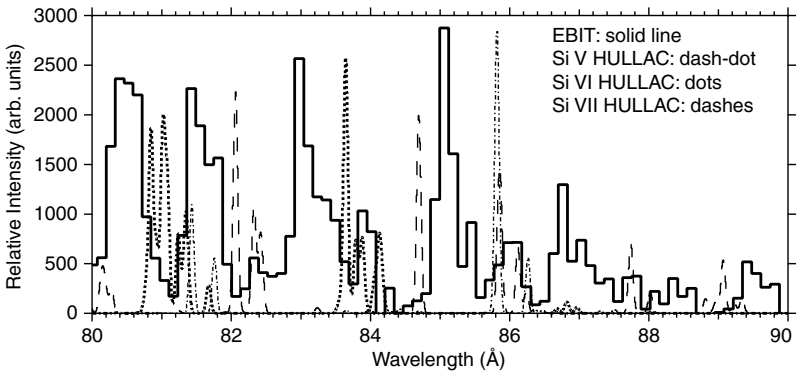

Fig. 1. Emission spectrum of silicon taken on EBIT-I at a beam energy of 300 eV, showing Si V, Si VI and Si VII. Synthetic spectra from HULLAC calculations for these charge states are overlaid to show the accuracy of calculations. The HULLAC spectra have been normalized to the strongest peak for each charge state.

tally determines which feature belongs to which ionization state. Even then it is very difficult. In an astrophysical plasma, where there are not only different charge states from one element but where ions from many elements are present, the task is clearly hopeless unless the wavelengths are well known.

We determined the wavelengths of most of the strongest lines in a given spectrum which were easiest to identify [5–7]. Tables 1–3 show the mean deviation of HULLAC calculations from measured wavelength values for neon-like through lithium-like ions of argon, sulfur and silicon. Although the closed-shell neon-like configuration

Table 1
Comparison of measured and predicted wavelengths for argon

Ion	n	$\delta\lambda$ (Å)	Range
Ar IX	10	0.125	0.048–0.196
Ar X	44	0.103	0.014–0.314
Ar XI	19	0.086	0.002–0.225
Ar XII	13	0.077	0.002–0.221
Ar XIII	11	0.120	0.021–0.237
Ar XIV	13	0.087	0.008–0.201
Ar XV	6	0.057	0.001–0.135
Ar XVI	7	0.012	0.001–0.022

$\delta\lambda$ is the mean difference between wavelengths measured on EBIT and predicted by HULLAC. Range is the smallest and largest deviation between experiment and theory for each ion. n is the number of lines compared for each ion.

Table 2
Comparison of measured and predicted wavelengths for sulfur

Ion	n	Mean $\delta\lambda$ (Å)	Range
S VII	10	0.257	0.135–0.426
S VIII	33	0.201	0.003–0.531
S IX	30	0.214	0.025–0.636
S X	51	0.171	0.011–0.526
S XI	36	0.116	0.010–0.341
S XII	20	0.087	0.013–0.212
S XIII	11	0.075	0.001–0.235
S XIV	13	0.037	0.000–0.125

$\delta\lambda$ is the mean difference between wavelengths measured on EBIT and predicted by HULLAC. Range is the smallest and largest deviation between experiment and theory for each ion. n is the number of lines compared for each ion.

Table 3
Comparison of measured and predicted wavelengths for silicon

Ion	n	Mean $\delta\lambda$ (Å)	Range
Si V	13	0.550	0.133–0.750
Si VI	15	0.332	0.093–0.636
Si VII	19	0.346	0.080–0.621
Si VIII	17	0.247	0.067–0.454
Si IX	9	0.266	0.060–0.587
Si X	14	0.206	0.061–0.421
Si XI	8	0.167	0.004–0.432
Si XII	16	0.030	0.005–0.096

$\delta\lambda$ is the mean difference between wavelengths measured on EBIT and predicted by HULLAC. Range is the smallest and largest deviation between experiment and theory for each ion. n is the number of lines compared for each ion.

might be expected to be easily modeled, we found the largest mean deviations in neon-like Ar IX, S VII and Si V, which ranged to over 500 mÅ. Such large differences make it unwise to rely on theoretical calculations to identify unknown lines in astrophysical plasmas. Calculations did better as the number of electrons decreased, and mean deviations were smallest in the one-valence-electron lithium-like Ar XVI, S XIV and Si XII. In particular, mean $\delta\lambda$ for the seven lines we measured of Ar XVI was 12 mÅ. It was 30 mÅ for the 16 measured lines of Si XII and 37 mÅ for the 13 measured lines of S XIV. As expected, the mean deviations also increase as Z decreases because the relative effects of electron–electron correlations increase.

3. Conclusion

Our laboratory measurements have produced wavelength catalogues for argon, sulfur and silicon. Analysis of magnesium is in progress. Using the empirical wavelengths together with spectral modeling calculations of line intensities enables reliable identification of many new astrophysically observed lines in *Chandra* and *XMM-Newton* spectra.

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